Mixed-Integer PDE-Constrained Optimization

Applied Mathematics Research for Exascale Computing

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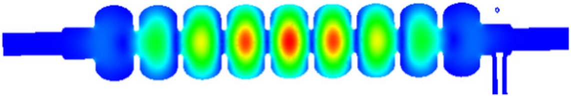
Mixed-Integer PDE-Constrained Optimization

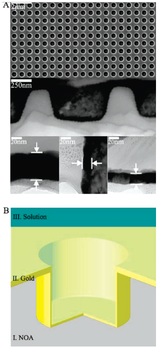
A new modeling paradigm

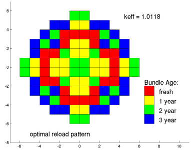
- Paradigm shift from forward simulations to design of complex structures
- Design of systems involving
  ... complex PDE simulations,
  ... uncertainty quantification,
  ... and discrete/continuous design parameters

Integrate maths, algorithms, and CS



Shape optimization of cavity for ILC
[Akcelik et al., 2005]

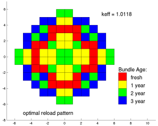




Applications of MIPDECO

A rich set of DOE application areas

1. Subsurface Design Applications
   E.g. remediation of contaminated sites, oil and gas extraction
   - PDE constraints model subsurface flow
   - Discrete design parameters model location/operation of wells
   - Uncertainties model the unknown subsurface
2. Operational planning for nuclear reactors: core-reloading
   - Neutron transport & fluid-flow equations
   - Discrete variables model fuel rod arrangement
   - Imperfect knowledge of fuel $\Rightarrow$ uncertainties

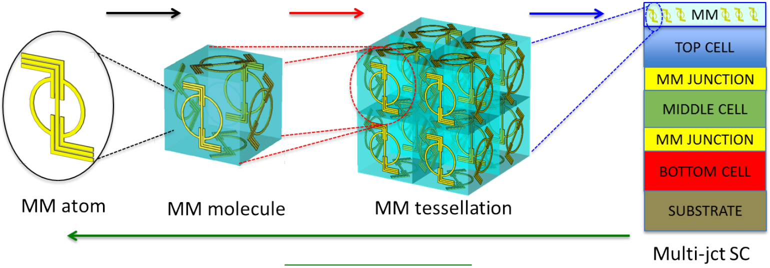


3. Accelerator design: Maxwell's equation plus discrete components, e.g. # arc & wiggler cells
4. Design of nano-materials for ultra-efficient solar cells ... next

MIPDECO for Design of Solar Cells

Goal: Design nonreciprocal coating: full transmission & absorption

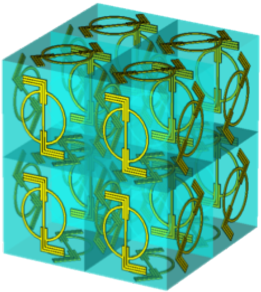
- Design meta-material (MM) coating for solar cells
- MM atom of given shape is assembled into molecule
- Typical crystal (layer of molecules) has 10-20 molecules width



- Maxwell's equation models electromagnetic response
- $0-1$ variables model orientation of atom on faces of molecule

MIPDECO for Design of Solar Cells

General form of Maxwell's equation



$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}_e, \;\; \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} + \mathbf{J}_m,$$
$$\nabla \cdot \mathbf{D} = \rho, \;\; \nabla \cdot \mathbf{B} = 0,$$

$$\begin{bmatrix} \mathbf{D} \\ \mathbf{B} \end{bmatrix} = \begin{bmatrix} \epsilon & \chi \\ \zeta & \mu \end{bmatrix} \begin{bmatrix} \mathbf{E} \\ \mathbf{H} \end{bmatrix} + \begin{bmatrix} \mathbf{P} \\ \mathbf{M} \end{bmatrix}$$

where $\epsilon = \epsilon(x)$ permittivity; μ permeability

Binary variables $z_{ijk} \in \{0, 1\}$ model orientation of MM atoms
$\Rightarrow$ construct permittivity and permeability tensors $\epsilon(x), \mu(x)$

$$\epsilon(x) \simeq \widetilde{\epsilon_{j,k}} = \sum_{i \in \mathcal{O}} z_{i,j,k} \epsilon_i \quad \text{and} \quad \sum_{i \in \mathcal{O}} z_{i,j,k} = 1$$

where ϵ_i is fixed permittivity of orientation i

Mathematical and Computational Challenges

Applications give rise to MIPDECO under Uncertainty

$$
\begin{aligned}
\underset{y(\gamma),u,z}{\text{minimize}} \quad & F(y(\gamma), u, z) \\
\text{subject to } & g(y(\gamma), u, z; \gamma) = 0, \ \forall \gamma \in \Gamma \\
& y(\gamma) \in \mathcal{Y}, \ u \in \mathcal{U}, \ z \in \mathbb{Z}^p \cap S,
\end{aligned}
$$

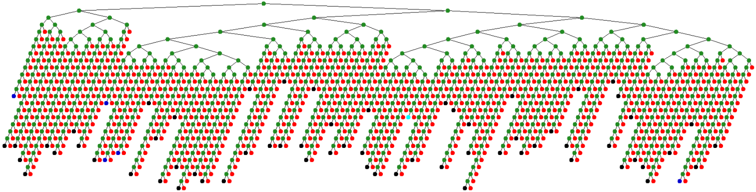
where

- $y(\gamma)$ state variables depending on random variables $\gamma \in \Gamma$
- u continuous design variables
- z integer design variables
- g describes PDE and boundary conditions
- $F(y(\gamma), u, z)$ is objective, e.g. maximize power of solar cells

Challenge I: Combinatorial Explosion

MIPDECOs generate huge search trees [Belotti et al., 2013]

- Each node in tree is PDE-constrained optimization
- Must take uncertainty into account
- $\{4 \text{ angles}\} \times \{6 \text{ faces}\} \times \{10\text{k cubes}\} = 24\text{k}$ binary variables
  Brute-Force Approach: assume billion PDECOs per second
  $\Rightarrow$ exascale machine would run longer than age of universe!



Must exploit hot-starts for re-solve ... solve millions of (N)LPs

Challenge II: New Algorithms & Math

A Simple Approach

$$\left\{ \begin{array}{c} \text{PICO [Eckstein et al., 2001]} \\ \text{MINOTAUR [Mahajan et al., 2011]} \end{array} \right\} + \left\{ \begin{array}{c} \text{PETSc} \\ \text{Trilinos} \end{array} \right\} \Rightarrow \quad \textbf{failure}$$

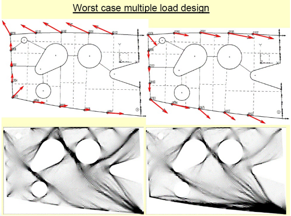
Need integrated algorithmic strategy, e.g.

- Tree-search techniques based on surrogate models
- Integrate multilevel combinatorial with multilevel PDE
- Optimization framework guides exploration of uncertainty
- Align algorithmic hierarchies with machine/storage hierarchies

... concerted effort worthy of DOE labs

New math challenges

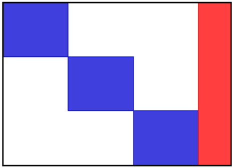
- Quality or bounds on surrogate models
- What is $\{0,1\}^{\infty}$? E.g. function space for topology optimization



Integrated Uncertainty Quantification

Sources of Uncertainty

- Errors in material properties (ϵ, μ)
- Manufacturing inaccuracies
- Numerical/modeling errors
- Errors from data measurements



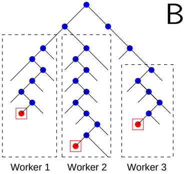
Combine PDECO with stochastic programming for UQ

- Design under UQ as two-stage stochastic MIP optimization
- First-stage variables are design variables
- Second-stage variables are solutions of stochastic PDE

$\Rightarrow$ Block-angular structure, where each block is PDE

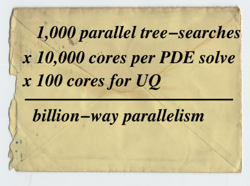
Goal: control uncertainty; dimension reduction; adjoint technology

Toward Billion-Way Concurrency



Back-of-Envelope Computation

- Asynchronous tree-search
- Linear solvers inside PDEs
- UQ block-structure



Opportunities for Exascale

- Tree-search loosely coupled solves with small communication
  - Readily scales to 1,000 parallel tree-searches [Goux and Leyffer, 2003]
  - Communicate bounds, new solutions, and sub-trees
- Parallel solvers for PDE-constrained optimization
  - Scalable linear algebra ... up to 150k cores (NEK5000)
- Scenario-based decomposition or UQ
  - Scales with number of scenarios (samples)
  - Some communication between scenarios

Hierarchy of concurrency $\Rightarrow$ multiplicative opportunities

Algorithm-Level Resiliency

Exascale systems likely to have shorter mean-time-to-failure
... check-point-restart no longer an option

Optimization Algorithms can be made resilient

- MIP tree-search: only check-point master node
- Trust-region or line-search provide algorithmic resilience
- Exploit multi-level hierarchy for smart check-pointing
- Stochastic programming (UQ) robust to node failures
- Resilient linear solves [Bridges et al., 2012]

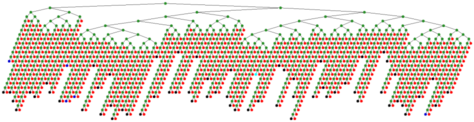
... exploit resilient algorithm design at all levels of hierarchy

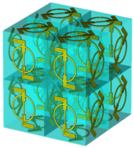
Summary and Discussion

Mixed-Integer PDE-Constrained Optimization

- Design of complex systems with discrete parameters under uncertainty
- Opportunity to tackle new, broader class of design applications
- Poses rich set of mathematical, algorithmic, and CS challenges
- Math and DOE applications "made for exascale"
    - Unlikely to tackle problems on smaller systems
    - Hierarchy of concurrency maps well to exascale systems
    - Integrates & combines existing DOE tools

… requires concerted & coordinated effort





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